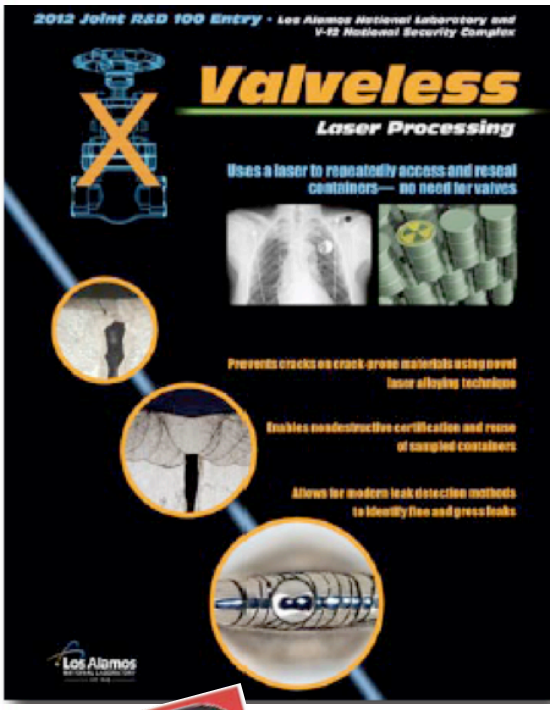
MST e-NEWS

August 2012

INSIDE

MST researchers win R&D 100 award



Materials Science and Technology researchers Tom Lienert and Martin Piltch (Metallurgy, MST-6) are recipients of a 2012 "R&D 100" Award from *R&D Magazine* for their work on Valveless Laser Processing, a technology that eliminates the use of valves in hermetically sealed containers (even those not designed for interrogation) by using a laser to access and reseal the containers. Also making significant contributions to the technology were MST-6's Jacob Sutton, Dave Alexander, Robert Forsyth Pallas Papin, and Tim Tucker.

Their award was one of four R&D 100 awards earned by the Laboratory this year. These awards honor the top 100 proven technological advances of the year, as selected by a group of *R&D Magazine*'s chosen judges.

"Congratulations to this year's R&D 100 award winners," said Energy Secretary Steven Chu. "The research and development at the Department of Energy's laboratories continues to help the nation meet our energy challenges, strengthen our national security and improve our economic competitiveness."

"These awards demonstrate the continued success of Los Alamos researchers and partners in defining the frontiers of innovation across a wide range of national security science," said LANL Director Charlie McMillan. "This innovation and creativity will drive the solutions to tomorrow's problems."

The unique laser-alloying technique prevents cracks on materials that are typically prone to cracking. Researchers can reseal containers by welding them with the alloy material, and then certify these seals to the highest standards. This allows nondestructive certification and reuse of sampled containers. The development eliminates the need for valves and their associated weight, volume, and material costs. It lowers process cost and duration because the technology can access, evacuate, backfill, seal, and leak test in one setup. Applications include environmental remediation (remotely accesses and reseals containers with known or unknown contents), nondestructive analysis (allows sampling, recertification, and reuse of containers typically analyzed by destructive means), and leak testing (enables modern leak detection on pacemakers and other implantable medical devices). In addition to Lienert and Piltch, award recipients include Jessie Nichols

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Worker Safety and Security Teams

WSST stands for worker safety and security team; the key word being "worker." Although one might think WSSTs are just another of the many "safety things" we are required to do and dismiss them as trivial, WSSTs are, however, an opportunity to have a say in how we treat safety and security at the Lab. This is what the "worker" in WSST means. We are a team run by the workers in collaboration with management.

In December 2005 Los Alamos National Security (LANS) was awarded the contract to manage and operate Los Alamos National Laboratory. As part of the proposal, LANS set as a goal attaining Department of Energy Voluntary Protection Program (VPP) Star Status. Star recognition is the highest achievement level in the VPP and recognizes outstanding safety and health programs. VPP's main tenant is that management and workers come together to solve long standing, as well as short-term, safety and health problems present in the everyday workplace. As part of working towards VPP certification, the institutional WSST was formed late in 2006.

The worker is the expert at how to improve safety and security in his or her workplace. These improvements may include easy access to needed tools, well-maintained parking lots and sidewalks, or repair and maintenance of the facilities in which we work. As workers we may be frustrated and discouraged at the perceived lack of interest in our workplace's condition and the difficulties in our ability to address these problems. We seem to be required to read more and more documents to address safety compliance, but have seen little participation in actually solving existing problems.
Our directorate's WSSTs actively try to solve these problems. ADEPS management is active and supportive, and while financial constraints limit what can be done to solve problems, it has been effective in solving many problems in the past few years. Below are some of the many accomplishments due to WSST involvement.

Problems solved due to solutions teams walk arounds include

- Emergency lights are in the process of being installed in a lab at MST. The lab is very dark with the lights off and would be dangerous in the case of a power failure
- Mystery circuit breakers in a lab were identified, supplying power for instruments in that lab
- A faulty plug in behind a glove box was discovered and repaired
- Electrical safety refresher courses were surveyed. The results were given to instructors in hopes that classes can be refurbished to better meet our needs.
- Crosswalk signage was placed in more obvious places at TA-53 to enhance safety.
- Trees that were intrusive to walkways have been trimmed. A dead tree in front of the Materials Science Laboratory was cut down after WSST intervention. It took further intervention to get it removed.
- Additional cell phone boxes placed at TA-3 in a timely manner
- WSST facilitated repair of exterior lighting along pedestrian path at TA-35 within 2 days.
- Coordinated with ice and snow removal teams to increase removal efforts in problem parking and pedestrian walk areas.
- A mess of ice and mud left in the government vehicle parking spots left after fire hydrant repair was cleaned up after WSST intervention.

These are just a few of the many accomplishments of the WSSTs in your directorate. We would like to add more to the list, which could be accomplished with more participation among the workers. Please get to know the WSST reps in your groups and work with them on problems that exist. They may be able to help you.

The photos on the next page are of your division reps. Can you match the name and face to your division? If you don't know the rep in your group, the face you see can tell you who he or she is. Get to know your group rep, or even better, become your group rep or alternate rep. With help from workers we can shed light on problems that need fixing at the worker level, and get some of them solved.

The ADEPS WSST

Take the

Take the 'Know your Worker Safety and Security Team rep'

QUIZ!

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KEY: A7, B4, C6, D3, E1, F2, G5

R&D 100 . . .

(Weapons Product Definition, W-11), Pete Pittman (76/W88, W-2), Marc Robbins and Wynn Christiansen (Applied Engineering Technology, AET-5), and Ken Nicklaus and Chris Hayes (Y-12 National Security Complex).

Since 1978 Los Alamos has won 124 of the prestigious R&D100 awards that celebrate the top 100 proven technological advances of the year as judged by *R&D 100 Magazine*. These technologies include innovative new materials, chemistry breakthroughs, biomedical products, consumer items, testing equipment, and high-energy physics.

Since 1995, winning innovations have returned more than $45 million in funding to Los Alamos in the form of Cooperative Research and Development Agreements, Work for Others, User Facility Agreements and licenses. More than 80 patent awards have been associated with winners with many more patents pending. More than 25 percent of LANL's commercial licenses and 35 percent of noncommercial licenses can be attributed to R&D 100 winners.

MST-7 researcher lends expertise to optical materials journal

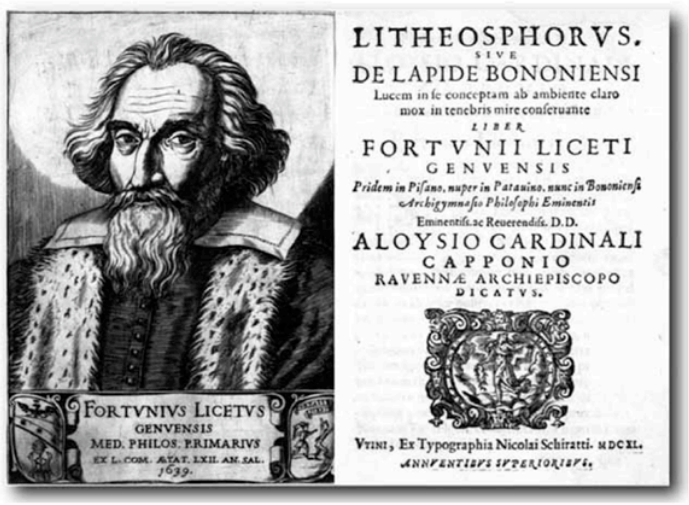
Markus Hehlen (Polymers and Coatings, MST-7) together with Philippe Smet and Dirk Poelman (Ghent University, Belgium) have edited a recent virtual feature issue on persistent phosphors that has been published in *Optical Materials Express* (www.opticsinfobase.org/ome/virtual_issue.cfm?vid=164).

Persistent phosphors can emit light long after the excitation has ended. Their most famous application is the myriad of "glow-in-the-dark" toys familiar to all.

The issue features peer-reviewed contributions from "Phosphoros 2011," the first international workshop on persistent phosphors held in Ghent, Belgium. The papers cover the wide gamut of persistent luminescence, ranging from the hundreds-of-years-old history of persistent luminescence all the way to the development of modern high-performance persistent phosphors. Elucidating the fundamental processes responsible for persistent luminescence is a particularly active area of research, and the mechanisms are still not fully understood in many cases.

Fifteen years ago, this field of research went through a revival with the discovery of bright and long-lasting luminescence in $SrAl_2O_4$:Eu,Dy by Matsuzawa et al [*J. Electrochem. Soc.* **143** 2670 (1996)]. Today, persistent phosphors emitting in red, green, and blue colors are available and find a variety of applications in emergency signage, toys, and consumer electronics. Los Alamos researchers are pursuing these phosphors for counterfeit detection and a number of global security applications.

17th Century



21st Century

Persistent luminescence is probably the first kind of documented luminescence. An early specimen showing persistent luminescence was the "Bologna stone," described in a book by Fortunius Licetus in 1640 [left, from J. Hölsä, Electrochem. Soc. Interface 18 42-45 (2009)]. Today, persistent phosphors primarily find application in emergency signage that does not require electrical power (right, from GloNation LLC, Falmouth KY).

Scripta Materialia ranks Los Alamos materials science paper one of hottest research papers

In the field of materials science, an article by four Los Alamos National Laboratory researchers ranked No. 16 as one of the most downloaded articles from the journal *Scripta Materialia* during October to December 2011.

Every three months, SciVerse ScienceDirect compiles the top 25 hottest research papers, as measured by the number of articles downloaded. The scientific database generates an overall list, as well as top 25 lists for specific subject areas and journals.

Jian Wang (Materials in Radiation and Dynamic Extremes, MST-8), Irene Beyerlein and Ruifeng Zhang (Fluid Dynamics and Solid Mechanics, T-3) and Timothy Germann (Physics and Chemistry of Materials, T-1) identified the nucleation mechanisms of dislocations from metallic interfaces by atomistic simulations.

The atomic structure of solid interfaces deviate significantly both structurally and/or chemically from that of the bulk crystals that they join. Hence it can be expected that the mechanically-driven processes by which an interface emits a lattice dislocation are different from those commonly associated with dislocation nucleation within the bulk. For grain boundaries, lattice dislocations usually nucleate from intrinsic or extrinsic grain boundary dislocations that have a Burgers vectors component lying out of the interface plane and the slip system of the freshly nucleated dislocation can be predicted by using dislocation theory and a Schmid factor analysis. For a flat, incoherent interface, intrinsic interface dislocations do not have a Burgers vectors component lying out of the interface plane, we found that the nucleation sites and the activated slip system correspond to regions with the most intense interface distortions, not solely determined by the crystallographic Schmid factor (Figure 1). In addition, the authors developed the single loop isolation method (SLIM), by which one loop nucleates in order to separating the effects of interface structure from those of loop-loop interactions, to determine the mechanics and energetics involved in the nucleation of an face centered cubic lattice dislocation from an atomistically flat interface. The results suggest that a flat, incoherent interface, free of extrinsic defects, can act as a dislocation source (Figure 2).

This work was supported by the Center for Materials at Irradiation and Mechanical Extremes, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number 2008LANL1026.

Reference: "Dislocation nucleation mechanisms from fcc/bcc incoherent interfaces," *Scripta Materialia*, **65** (11), 1022-1025, (2011).

Technical contacts: Jian Wang and Irene Beyerlein

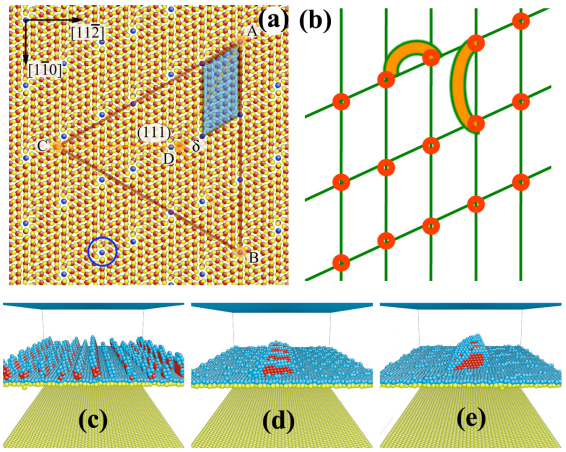


Figure 1 (a): Atomic structure of Cu/Nb interface. Three sides of the triangle indicate the traces of three glide planes on the interface plane. The blue sphere represents the center of intense interface distortions, which correspond to the intersection of interface dislocations that are illustrated by the green lines in (b). (c)-(e) shows the nucleated lattice dislocations from interfaces with respect to different stresses, that are along the line of interface dislocation and initialize at the intersections. Only three slip systems out of nine slip systems in Cu are activated, implying the strong correlation of interface structure with the selected slip systems.

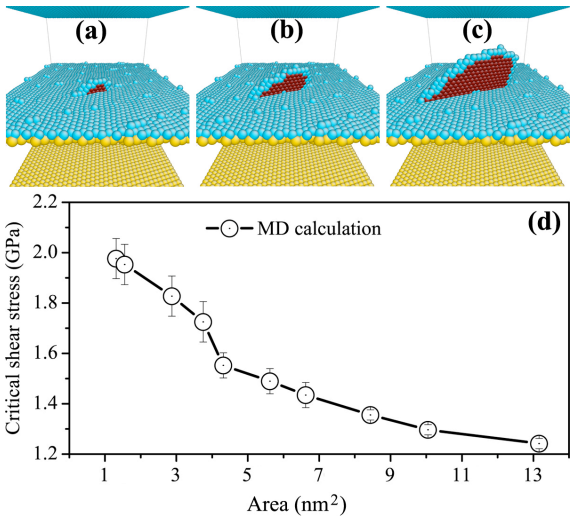


Figure 2: Using the SLIM method, (a)-(c) show the nucleation and growth of a single Shockley partial dislocation loop as a result of in-plane tension; (d) The critical shear stress to stabilize a dislocation loop as a function of dislocation loop size. Compared with the nucleation stress in bulk, the low shear stress (less than 2.0 GPa) implies that a flat, incoherent interface, free of extrinsic defects, can act as a dislocation source.

A novel approach to experimental studies of fission gasses in materials prospective for nuclear energy applications

Xenon (Xe) is one of the major gas elements produced during nuclear fission. It has long been known that Xe accumulation in the fuel pellet and Xe release to the plenum are detrimental to the fuel performance and safety and, therefore, must be well understood and controlled. Considerable theoretical and modeling efforts have been recently undertaken to clarify Xe diffusion mechanisms and understand the effect of Xe–filled bubbles on thermal transport in UO_2–based fuels. However, lack of reliable experimental data substantially impedes verification of modeling results for development of predictive nuclear fuels codes.

For verification of modeling results, testing of UO_2 samples with Xe concentration spanning from a fraction to a few of atomic percent (at.%) must be performed. Obtaining conventional UO_2 samples containing a few at.% of Xe accumulated in-pile is not possible without years of irradiation in a reactor. A major difficulty in interpretation of experimental data obtained from reactor irradiated UO_2 resides in the multitude of processes simultaneously taking place. Among which are: variation of radial fuel temperature and stoichiometry, microstructural changes, generation of point and extended defects, accumulation and migration of fission products with different chemical states.

Los Alamos scientists demonstrated that the ion beam assisted deposition (IBAD) technique can be utilized to produce reference UO_2 material with controllable Xe-filled bubble morphology, which closely resembles the one produced in a reactor irradiated fuels[1]. The basis for IBAD is a combination of film deposition with simultaneous low energy ion bombardment of the growing film surface. The UO_2<Xe> films were fabricated by electron beam evaporation of depleted UO_2 source material and bombardment with 1keV Xe+ ions. Under such conditions the range of Xe ions into UO_2 is only 2 nm. Even though the penetration depth of Xe is very shallow and the solubility is null, some of the Xe atoms are trapped in the sample. Films with Xe concentration up to 4 at.% can be readily produced by the IBAD method[2].

Fig. 3a shows high magnification transmission electron microscopy (TEM) images obtained from a UO_2<1.46 at.% Xe> film annealed at 1000 °C for 3 hours. Before annealing the film contains large density of void-type features with an average diameter ~ 6 nm. These voids were filled with Xe prior to the TEM foil preparation. After annealing, the void density is reduced dramatically and the diameter of the voids increased up to ~ 30 nm. The morphology and dimensions of the voids in IBAD samples closely resemble images obtained from reactor irradiated UO_2-based fuels.

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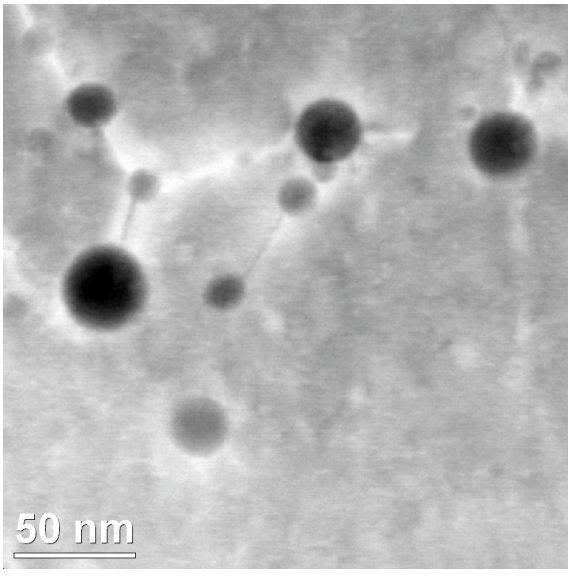

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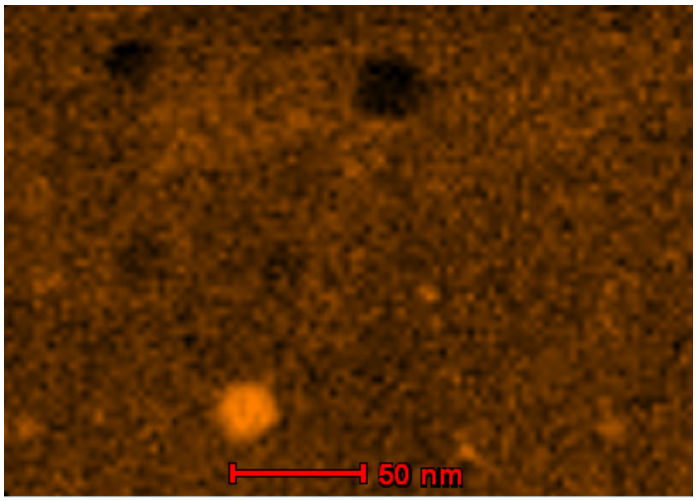

b

Figure 3: Scanning TEM (a) and Xe atomic distribution measured by EDXS (b) obtained from UO_2 film synthesized by the IBAD method and subsequently annealed at 1000 °C for 3 hours. The as deposited film contained 1.46 at. % of Xe atoms. The orange spherical feature represents a Xe-filled bubble.

Novel approach . . .

It is worth pointing out that it is very difficult to observe intact Xe-filled bubbles by the TEM method. A TEM foil must be transparent for the probing electron beam and therefore a very thin foil has to be produced. For UO_2 TEM analysis, the thickness of the foil must be a few 10's of nanometers. Thus during the foil preparation, the majority of Xe atoms aggregated into bubbles will escape from the sample. Consequently, a bubble initially filled with Xe will appear in a TEM image as an empty void. Xe-filled bubbles whose dimensions are smaller than the TEM foil thickness might stay intact and therefore might be possible to observe. Elemental mapping, shown in Fig. 3b, displays that one of the Xe-filled bubbles with diameter ~ 20 nm remained intact and the rest are just empty voids.

The value of such synthetic UO_2<Xe> samples is that fission gas introduction is separated from the various effects attendant to the fission process. The new technique offers the opportunity to develop a radiation-free, composition-controlled, systematic approach to elucidating the underlying physics of gas behavior in nuclear materials.

This concept was conceived under F^3 MaRIE influence and initial support was obtained from LDRD reserve funding. This work is currently supported by DOE NE Fuel Cycle R&D program (K. McClellan, MST-8)). Researchers include Igor Usov (MST-7), Robert Dickerson, Patricia Dickerson (both MST-6), Marilyn Hawley (MST-7), and Darrin Byler (MST-8). This work supports the Lab's Energy Security mission area and the Materials for the Future science pillar.

Technical contact: Igor Usov

[1] I.O. Usov, J.Won, D.J. Devlin, Y.-B. Jiang, J.A. Valdez, K.E. Sickafus "A novel method for incorporating fission gas elements into solids," *J. Nucl . Mater.* **408** 205 (2011).
[2] I.O. Usov, R.M. Dickerson, P.O. Dickerson M.E. Hawley, D.D. Byler, K.J. McClellan, "Thin uranium dioxide films with embedded xenon," submitted *J. Nucl . Mater.*

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To submit news items or for more information, contact Karen Kippen, EPS Communications, at 606-1822, or kkippen@lanl.gov.

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HeadsUP!

UI Division Call Center activated

Utilities and Institutional Facilities (UI) Division has activated a Call Center to help improve and more closely work with tenants to meet their maintenance and facility operation needs. The call center provides another method for requesting services and is a communication tool to clarify delivery expectations that UI can meet and deliver. The Call Center number is 667-2488. Through the UI Call Center, employees can

- make requests from UI for reporting facility related problems
- requesting routine maintenance or repairs
- requesting office furniture or equipment moves, etc.

Employees can still make requests through the Facility Request System. Establishment of the call center resulted from feedback provided through a survey UI conducted earlier this year. "The call center will help improve our service delivery. We encourage our customers to contact the call center to inquire on status or expected delivery dates of when work will be performed," said Martin Aguilera, MSS-UI maintenance manager. Questions? Contact Aguilera t 5-4720.

Proper operation of government vehicles

LANL's fleet is a critical resource to the Laboratory. As summarized below and detailed in the Property Management Manual, there are stringent requirements that must be followed when using a Los Alamos-owned, -rented or -leased motor vehicle:

1) Vehicles may only be used for official purpose by LANL, subcontractors, and other government personnel. 2) Operators are allowed to use government vehicles for official travel (in lieu of renting a vehicle), when authorized by a group level manager or higher. 3) In rare circumstances, when an employee must take a government vehicle home, a fully executed Government Vehicle Work-to-Home Approval form is required. Use of the vehicle overnight remains strictly limited to official government business (not commuting). It is not to be used to transport family members or personal items. A new form is required for each trip. More information regarding the proper operation of government vehicles is at the above referenced website link, or contact LANL Property Management at lanlproperty@lanl.gov or 5-3230.